The work was performed at the Combustion Research Facility, Sandia National Laboratories, Livermore, CA. Financial support was provided by the U.S. Department of Energy, Vehicle Technologies Office. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Gasoline Combustion Fundamentals

Presenter: Isaac Ekoto
Sandia National Laboratories

2019 DOE Vehicle Technologies Annual Merit Review
Washington, DC
June 11, 2019 – 9:30 a.m.

Program Managers: Michael R. Weismiller & Gurpreet Singh
U.S. DOE Office of Vehicle Technologies

Project ID: ACE006

This presentation does not contain any proprietary, confidential, or otherwise restricted information

Overview

Timeline

- Project provides fundamental research supporting DOE/industry advanced engine development projects.
- Project directions and continuation are evaluated annually.

Barriers identified in 2018 ACEC Control Roadmap

- Evaluate robust ignition systems needed at lean/dilute and boosted conditions to reduce combustion variability
- Inadequate understanding of low-temperature combustion (LTC) fundamentals for a range of conditions
- Strategies and technologies for controlling mixed-mode operation need continued improvement

Budget

- Project funded by DOE/VT
- FY19 funding: $930K
- FY18 funding: $920K

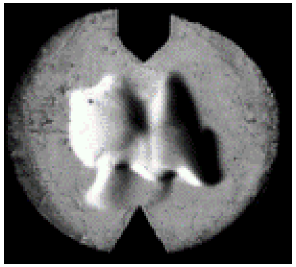
Partners

- Project lead: Isaac Ekoto, Sandia National Laboratories
- Industry/Small Business Partners:
  - GM, Ford, John Deere: technical guidance
  - Transient Plasma Systems Inc.
  - Esgee Technologies
  - Tula Technologies
  - 15 Industry partners in DOE Working Group
- University/National Lab Collaborators:
  - Oak Ridge National Laboratory: 3D printed pre-chamber
  - Argonne National Lab: Low-temperature plasma modeling
  - U. Orléans (France): Effects of ozone addition on LTC
  - Michigan Technical University: LTP measurements

Relevance

Motivation

Improved ignition can enable a 25% increase in engine efficiency, lower pollutant emissions, and more reliable cold-start, <u>but requires improved understanding and robust modeling approaches to optimize</u>



Barriers and Associated Objectives

- First-principles plasma discharge modeling—needed for accurate engineering ignition models for conventional & advanced igniters—is in its infancy and not yet well-validated
  - Energy deposition (where, how much, and what mechanisms dominate?)
  - Radical formation (what radicals and how much?)

Discharge

- Discharge-to-ignition transition is the limiting factor for dilute/lean combustion concepts
  - Compare dilute/lean ignition limits extension with transient plasma ignition (TPI)
  - Measure early flame growth rates for conventional spark and compare to TPI

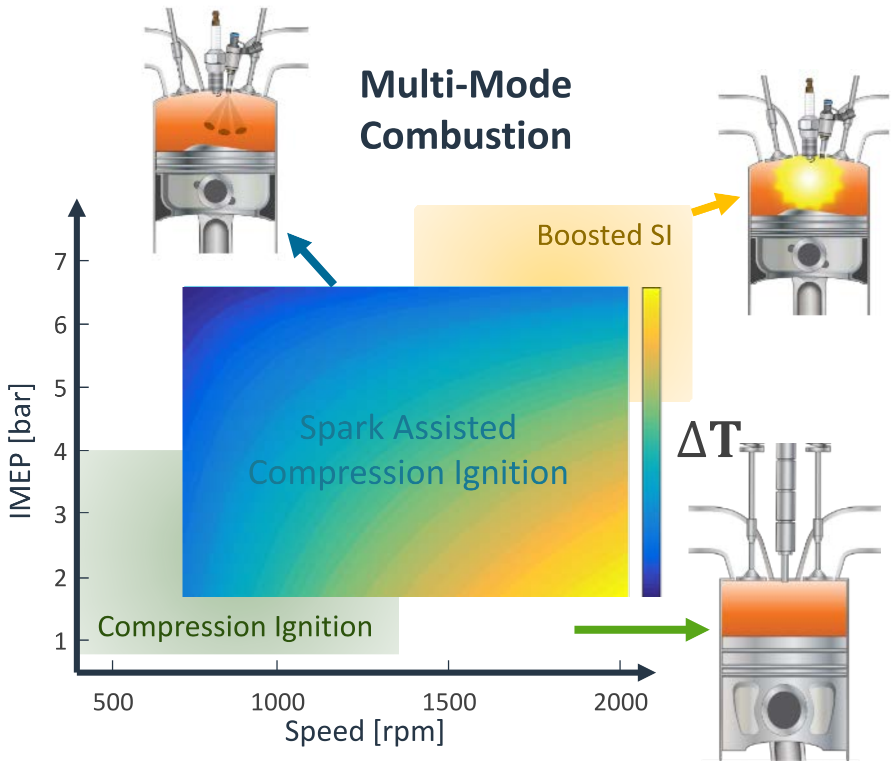
Ignition

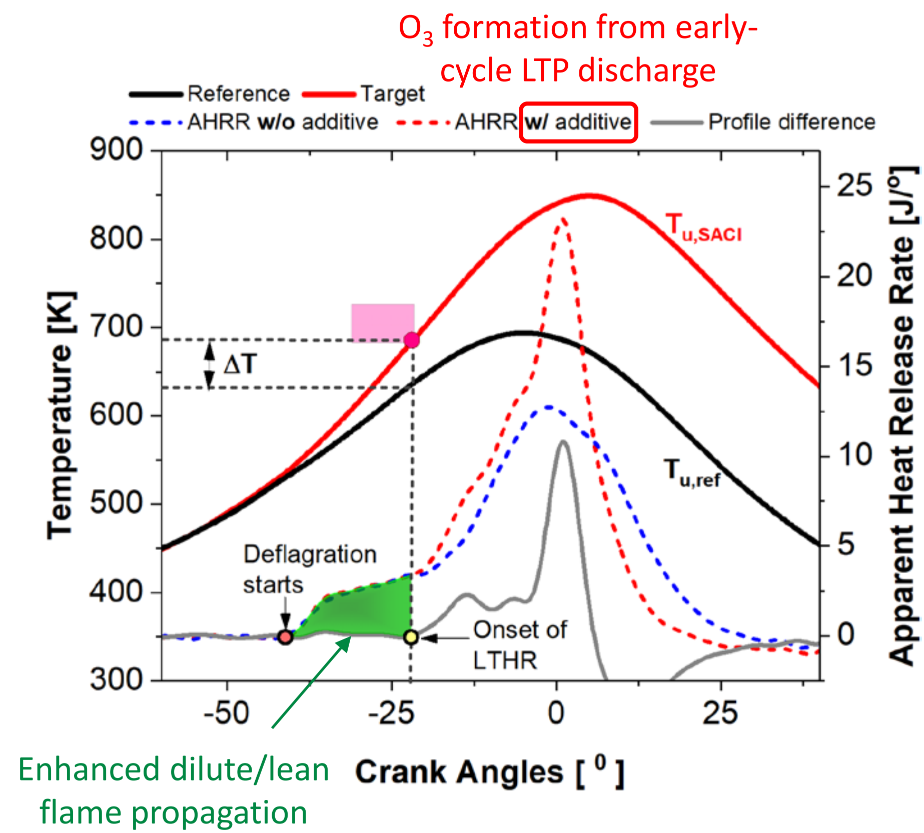
- New modes of operation are needed to fully realize the benefits of conventional and advanced igniters
  - Spark assisted compression ignition (SACI) with ozone (O_3) addition
  - Expanded spark ignition (SI) dilution tolerance with TPI

Engine Combustion

Approach

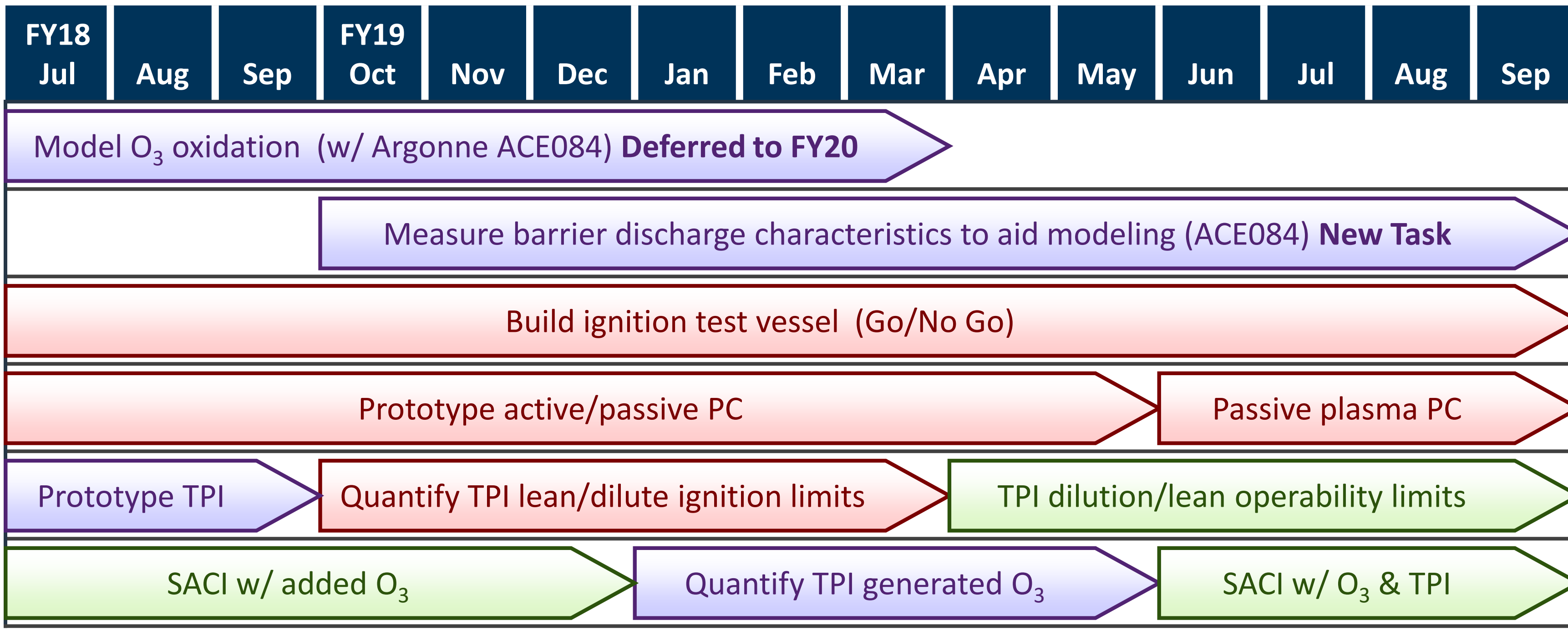
Example: Advanced ignition can enable O_3 enhanced SACI
(likewise benefits dilute/lean SI & enables spark retard for boosted SI)



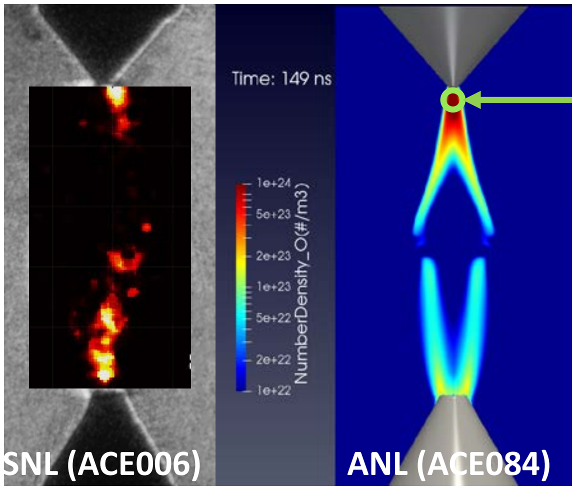


Project couples unique capability to design & fabricate custom igniters and measure ignition quantities of interest with complementary engine testing

FY19 Milestones



Accomplishments – FY18: Discharge & Engine Combustion



Scarcelli, et al, *Plasma Sources Sci T* 27(12) 2018

TPI Discharge Fundamentals

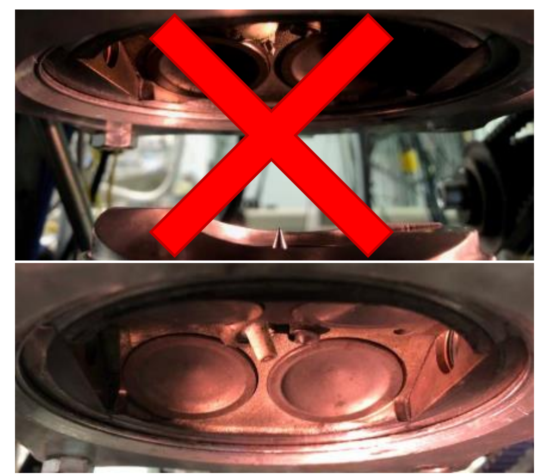
- Good qualitative & quantitative agreement between measurements and complementary simulations (ACE084) for a canonical geometry

	Experiment	Simulation	Experiment	Simulation
Test Condition	O (1/cm^3)		T (K)	
14.4 kV, 1.5 bar	1.3 x 10^{18}	0.9 x 10^{18}	779	770
19.2 kV, 2.0 bar	2.1 x 10^{18}	1.8 x 10^{18}	1094	938

- Modeling insights used to develop pulse strategies & new igniter geometries (e.g., electrode, voltage, frequency, pulse number)

TPI Engine Testing

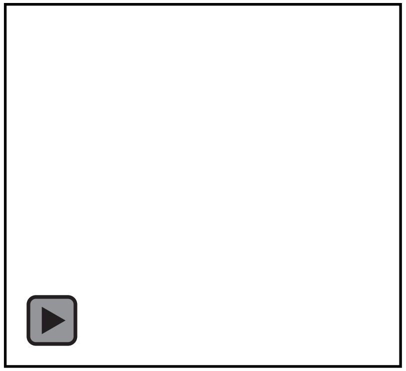
- Goal: Early-cycle O_3 formation; late-cycle ignition
- Variable pin-to-pin (P2P) & groundless dielectric barrier discharge igniter (GBDI) electrodes
- P2P geometry rejected due to complex control strategy, piston heat transfer issues, and early-cycle arc to the injector
- **Promising GBDI results, but pulse waveform optimization was needed to minimize arc transition (see Technical Backup Slide 5)**



Summary: We know a lot about discharge characteristics but engine tests failed largely because we do not understand ignition transition mechanisms

Accomplishments – Ignition

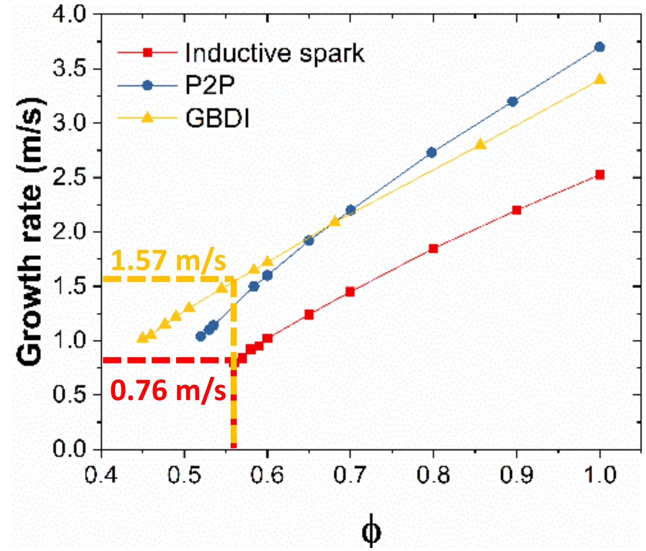
1.3 bar, 343 K, propane/air

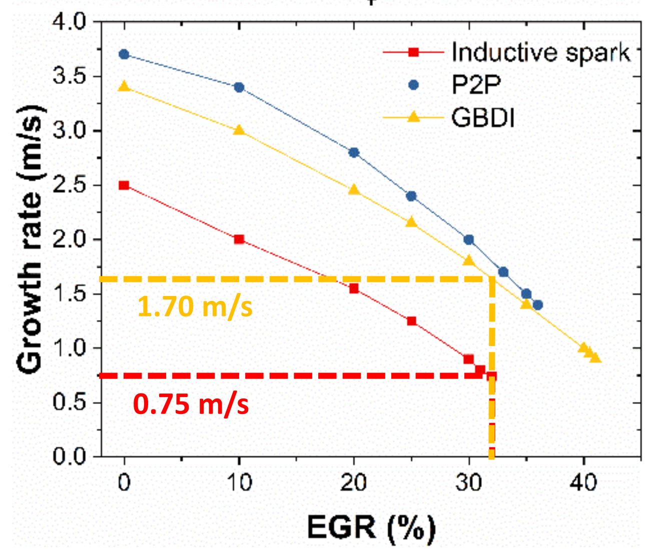


$\phi = 0.56$, 93 mJ

$\phi = 0.52$; 97 mJ

$\phi = 0.45$; 157 mJ





TPI Ignition Testing

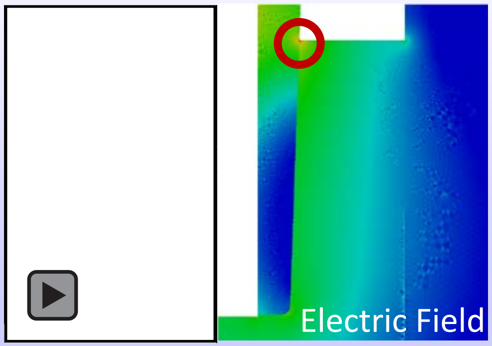
- Igniters tested: Inductive spark, TPI (P2P, GBDI)
- TPI ignited much more dilute/leaner mixtures relative to inductive spark with comparable secondary energies
- Unusual GBDI ignition behavior due to possible surface streamer interactions at the lean limit ($\phi = 0.45$)
- Faster TPI flame growth rates relative to inductive spark
  - ***More than double** for the leanest ($\phi = 0.56$) and most dilute mixtures (EGR = 32%)*

Impact: Results highlight new physics (i.e., surface streamer ignition) that may be leveraged to further expand dilute/lean ignition limits

Accomplishments – Discharge

GBDI Surface Physics

- Surface chemistry evidence
- Strongest electric fields at contact surfaces (ACE084)

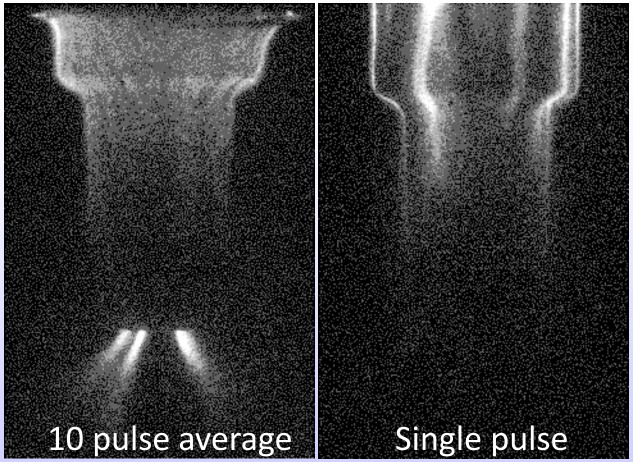


GBDI Electrode Redesign

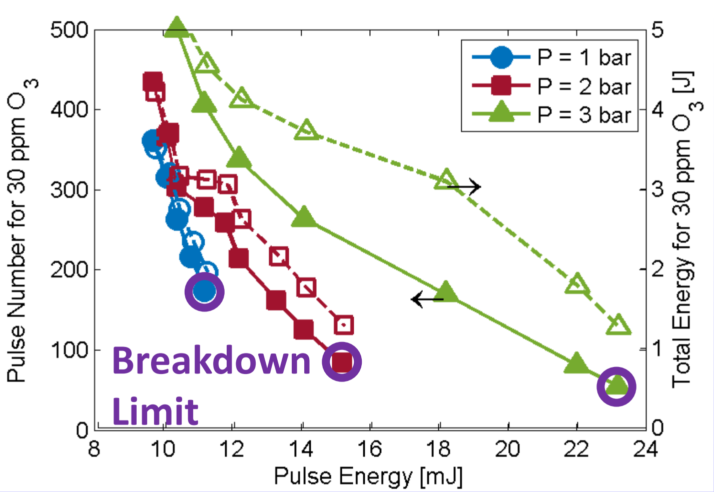
- v1.1: Increased surface area

  – Discharge/ignition unaffected
- v1.2: Inhibit breakdown

  – 10x more luminous streamers
  – Breakdown virtually eliminated
  – **Lower lean limit: ϕ = 0. 45 → 0.41**



GBDI v1.1 **GBDI v1.2**



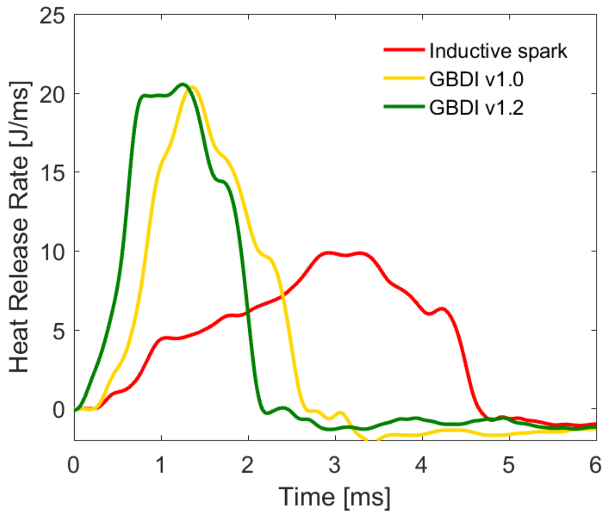
GBDI v1.0 O_3 Formation

- Non-linear O_3 production w/ pulse energy
  – Higher energies limited by breakdown
- Best production eff. w/ high pulse energy & low pressure
  – 93 mJ: theoretical limit for the *0.55 L* cylinder
  – Optimal engine production should be early in the cycle
- **GBDI v1.2 could help by limiting low pressure breakdown**

Impact: New understanding used to identify and model optimal igniter design features

Accomplishments – Ignition & Engine Combustion

1.3 bar, 343 K, propane/air, ϕ = 0.6



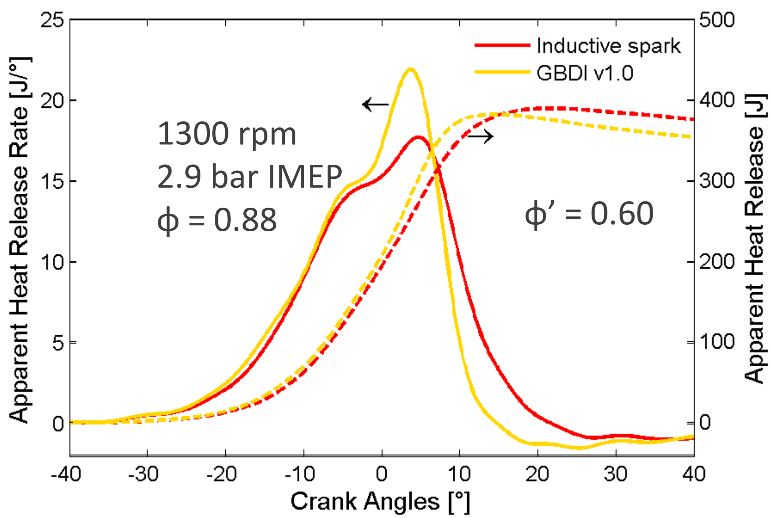
GBDI v1.2 Ignition Behavior

- Peak burn rates ***doubled*** for GBDI v1.0 and total burn duration halved
- Further acceleration of early burn rates w/ GBDI v1.2
  - Very repeatable combustion (beneficial for cyclic stability)
- Clear benefit for TPI in quiescent environments

  Does this translate to the engine?

GBDI Engine Testing

- Goal: Find dilution limit for GBDI v1.0 and spark
  - Unable to test GBDI v1.2 in time for this presentation
- GBDI v1.0 expanded dilution tolerance limits by enabling additional spark advance
- Faster early stage heat release led to more end-gas auto-ignition and shorter burn durations

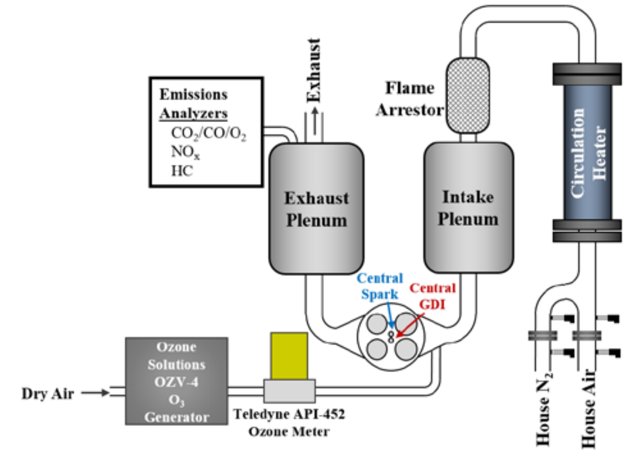


Takeaway: GBDI provides robust early flame behavior that enables faster engine combustion at dilute/lean conditions

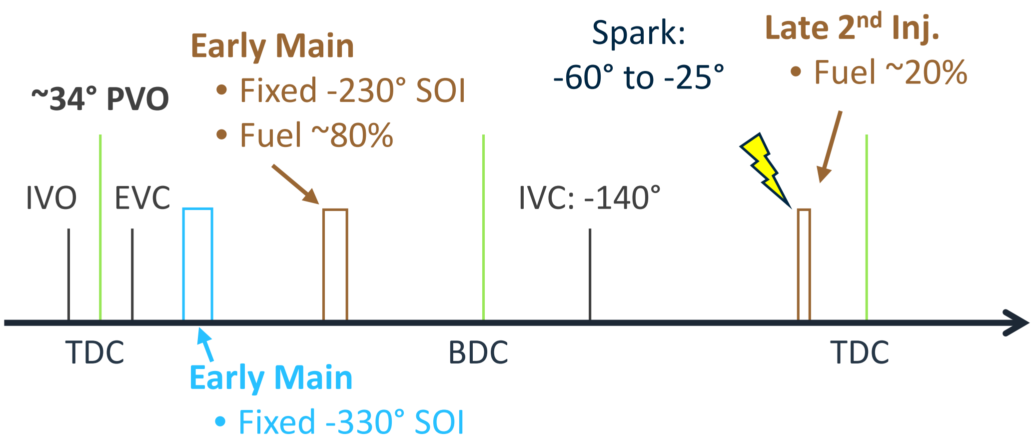
Accomplishments – Engine Combustion

O_3-Enhanced Kinetically Controlled Combustion

- **FY18:** Trace O_3 promotes low-temperature heat release (LTHR), which reduces intake temperature requirements for kinetically controlled strategies
  - Leverages igniter ability to create in-cylinder O_3
- **FY19 Goal:** Use O_3 to expand the range of part-load ***homogeneous*** and ***partially stratified*** SACI engine combustion strategies

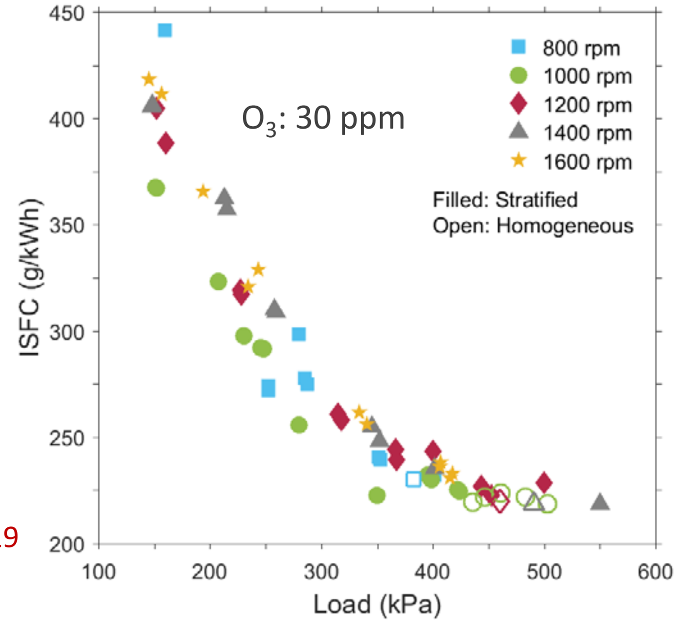


Combustion Mode	O_3 enhanced SACI
Engine Design	Spray Guided
Injector	Central VCO
Displacement [L]	0.55
Stroke/Bore	1.11
Compression Ratio	13
Intake Pressure [bar]	1
Exhaust Pressure [bar]	1.05
Intake Temperature [°C]	**42 – 80**
Intake O_3 Conc. [ppm]	**30 – 50**
Engine Speed [rpm]	**800 – 1600**
Equivalence Ratio	0.27 – 0.55
IMEP [bar]	**1.5 – 5.5**
Fuel	RD587

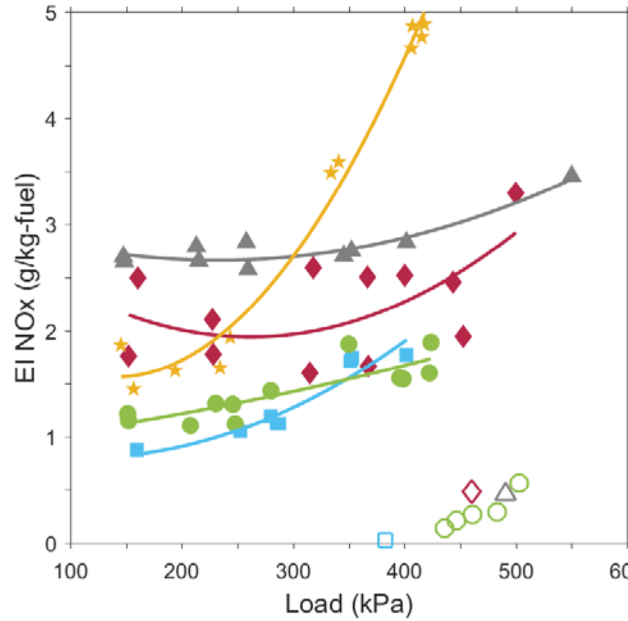


Expectation: O_3 addition will improve efficiency & reduce pollutant emissions through more stable combustion w/ less stratification

Accomplishments – Engine Combustion



Biswas & Ekoto,
SAE PF&L, Aug 2019



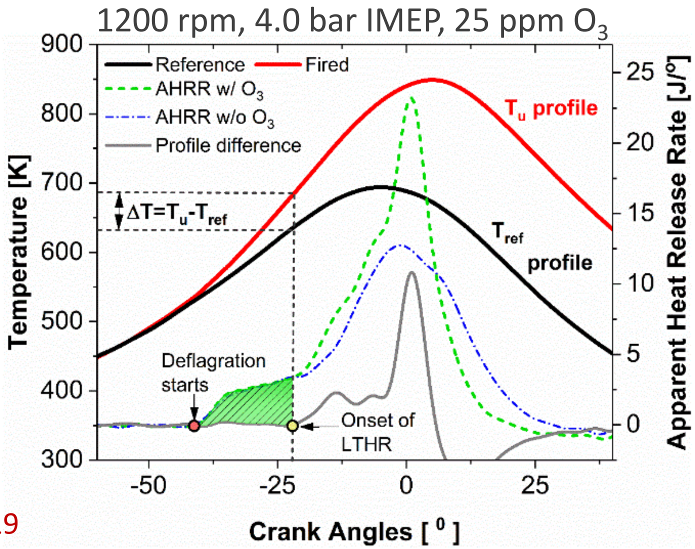
Biswas & Ekoto,
SAE WCX, Apr 2019

O_3-Enhanced SACI

- ***Partially Stratified Operation***
  - ↑ Robust speed/load range
  - ↑ 9% lower indicated specific fuel consumption (ISFC) w/ O_3 at lowest loads
  - ↓ Problematic nitrogen oxide (NOx) & particulate matter (PM) emissions
- ***Homogeneous Operation***
  - ↑ Similar efficiency to the partially stratified strategy
  - ↑ Ultra-low PM/NOx emissions
  - ↓ Does not work well at lower loads and higher speeds

Impact: O_3-addition alone greatly benefits SACI emissions & efficiency

Accomplishments – Engine Combustion



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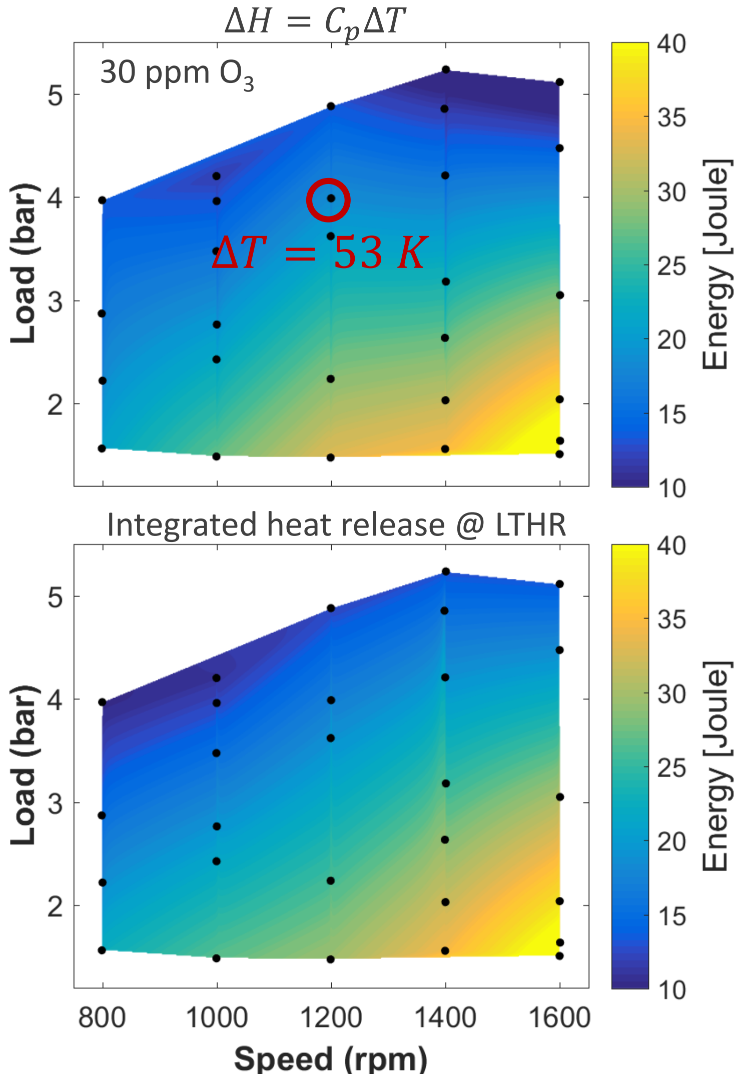
SAE PF&L, Aug 2019



O_3-Enhanced *Partially Stratified* SACI

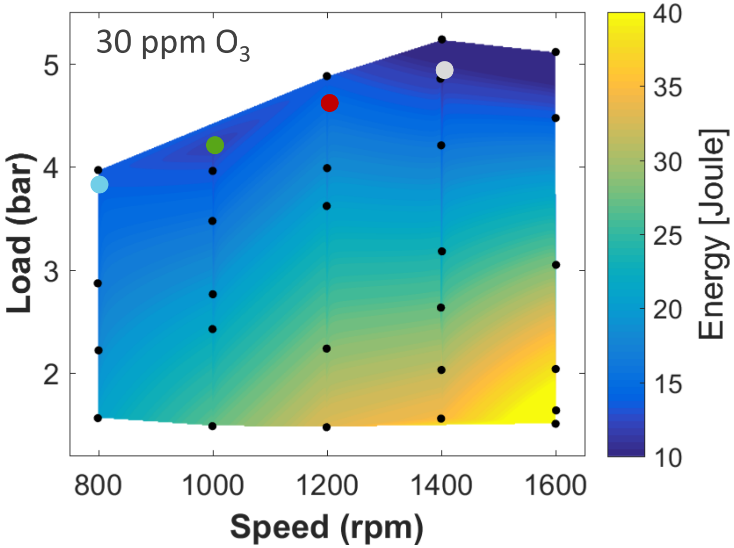
- End-gas auto-ignition proportional to added O_3
  - Decreased effectiveness with increased engine speed
- End-gas ΔT required for optimal auto-ignition increases with higher engine speeds & lower loads
- Good match between integrated heat release to LTHR onset and temperature difference methods

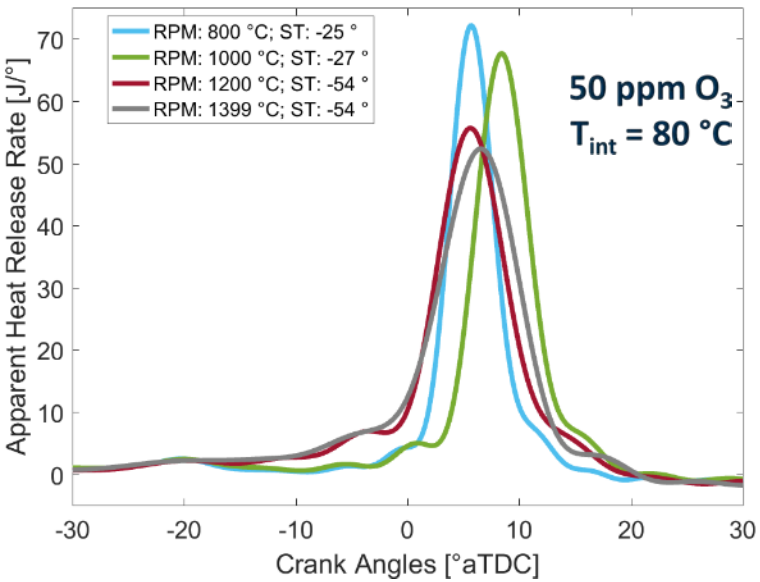
Impact: Conceptual model of end-gas energy requirements will enable development of a simplified modeling framework

Accomplishments – Engine Combustion

O_3-Enhanced *Homogeneous* SACI

- Lower loads are more difficult to achieve relative to ***partially stratified*** SACI
  - Intake temperature (80 °C) and O_3 concentration (50 ppm) were both increased
- Weak deflagration from highly dilute mixtures leads to negligible end-gas temperature increase

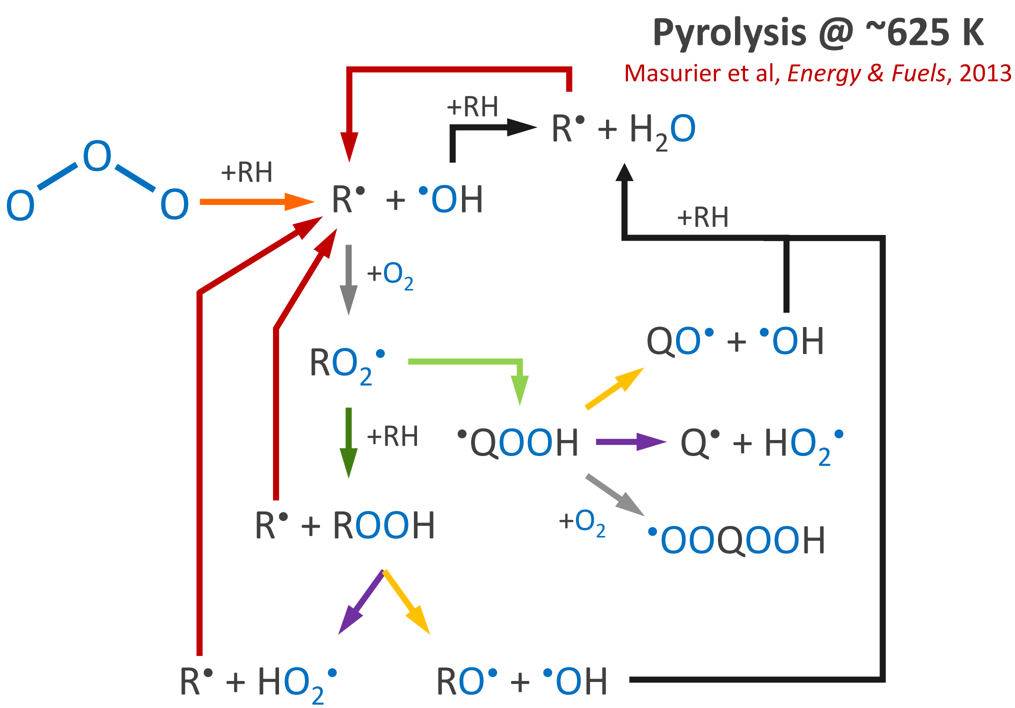


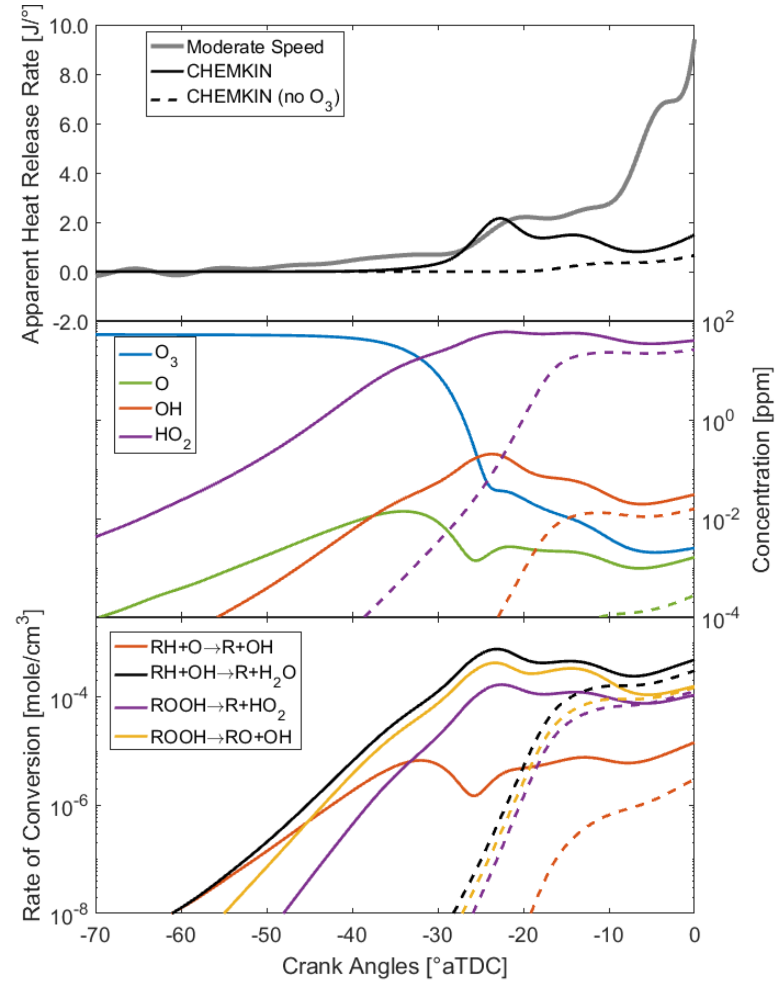


- Virtually all heat release from auto-ignition
- Low speed conditions (< 1200 rpm) not sensitive to spark advance
  - Large spark advance needed for higher engine speeds (1400+ rpm)

Impact: Results show stronger early deflagration periods are needed to promote lower load end-gas auto-ignition – clear synergy with TPI research

Accomplishments – Engine Combustion





Biswas & Ekoto, SAE WCX, 2019-01-0966

O_3 impact on LTHR Chemical Pathways

- O_3 pyrolysis depends on temperature & composition
- Fuel hydrogen abstraction by atomic oxygen ($O^\bullet$)
- Chain branching reactions form more alkyl radical ($R^\bullet$) and hydroxyl ($OH^\bullet$)

Impact: Explanation of O_3-enhanced LTHR kinetics enables identification of fuel molecules that will be most positively impacted by O_3 addition

Responses to Previous Year Reviewers' Comments

Q1,4,6 R1-5: "concerns with the current approach for the turbulent jet ignition (TJI) studies"

Response: Thank you for the valuable feedback. The points expressed by all reviewers that the PC work as proposed lacks relevance to production systems are well-taken. Accordingly, we propose merging the PC with ongoing TPI research to explore whether expanded dilution tolerance limits with TPI can enable ultra-lean/dilute PC operation without external fueling.

Q1 R1: "consider how more conventional ignition system technology compares to these advanced systems"

Response: Another excellent suggestion. This year we benchmarked conventional SI to TPI systems, but we also see value in more fundamental examinations of conventional SI systems to compare phenomenological aspects with those of advanced systems and to advance modeling of conventional systems.

Q2 R1,4,5: "more emphasis or results from engine tests"

Response: We again agree with the reviewers that it is important to have engine results for this project as a way to evaluate igniter performance. We caution that there still is a need for a mix of discharge and ignition experiments to quantitatively measure relevant fundamental phenomena, as these data are used to develop/validate complementary modeling efforts (ACE084).

Q3,6 R2,4,5: "surprised there is no collaboration with Esgee Tech."
"not enough collaboration w/ ignition system suppliers"

Response: Through Argonne (ACE084), we collaborate extensively with Esgee (4 journal pubs); not including them as a collaborator was an oversite on our part. While we converse with ignition system suppliers, our relative lack of cooperative research is mainly due to our focus on alternative ignition systems and the suppliers' reluctance to reveal too many details about their corresponding pre-production systems. With a renewed focus on more conventional systems, we expect this to be less of an issue. We also continue outreach concerning more advanced systems to find ways that we can leverage our capabilities to help answer important questions (e.g., O_3 generation and associated impact on engine combustion)

Collaboration and Coordination with Other Institutions

- National Laboratories
  - **Argonne National Laboratory (ACE084):** shared validation data in support of ignition modeling and pre-chamber hardware development
  - **Oak Ridge National Laboratory:** exploratory 3D printing of pre-chambers (microfluidic fueling)
- Automotive OEM and Suppliers
  - **General Motors (ACE121):** quarterly technical updates, ignition discussions, data sharing (e.g., heat release, O_3 profiles), research guidance, DSF and SG2 head hardware support
  - **Ford:** biannual technical updates, research directions, operating conditions
  - **John Deere:** hardware safety guidance, technical exchange on O_3 assisted combustion
  - **Federal Mogul:** preliminary cooperative research discussions
- University
  - **U. Orléans:** rapid compression machine testing to better tune O_3 oxidation kinetic models (joint publication at upcoming PFL meeting in Kyoto)
  - **Michigan Tech:** processing of atomic oxygen laser induced fluorescence data
- Small business
  - **Transient Plasma Systems Inc.:** data/hardware sharing, pulse generator support, DOE SBIR Phase II proposal submitted to evaluate different GBDI electrode configurations
  - **Tula Technologies:** guidance on engine head modification guidance to enable cylinder deactivation; plans for in-cylinder temperature and cycle resolved PM/PN measurements
  - **Esgee Technologies:** Joint publication of 4 papers on multi-physics modeling of nanosecond LTP
  - **Knite Inc.:** preliminary cooperative research discussions
- DOE Working Group:
  - Shared research results & insights at DOE's Advanced Engine Combustion project review meetings

Remaining Challenges and Barriers

- **Measurements of local plasma energy transfer needed (both conventional spark & LTP)**
  - Particular emphasis on influence spark deflection/re-strikes from cross-flows
- **GBDI holds promise as an advanced igniter, but optimal design features are unclear**
  - What factors influence surface ignition (e.g., curvature, anode/insulator thickness, materials)?
  - What are possible O_3 production yields (i.e., best design factors, sensitivity to fuel/EGR)?
  - Does GBDI still work at elevated pressures?

- **Unknown plasma-to-flame transition mechanisms (esp. at lean/dilute conditions)**
  - How does this plasma-to-flame transition work on a fundamental level? (Applies to both SI & LTP)
- **Factors that influence conventional SI flame growth rates for dilute/lean combustion**
  - What makes TPI flame propagation so fast?
  - Can conventional spark ignition be modified to replicate faster TPI growth rates?

- **Factors that limit spark retard (e.g., for cold-start catalyst light off)**
- **GBDI durability and interference issues with combustion chamber (e.g., valves)**
- **O_3-enhanced SACI using only GBDI**
  - Do vessel results translate to engine?

Proposed Future Research

- **Global and local measure of discharge energy deposition (conventional spark and LTP)**
  - Modify new ignition test vessel (see Technical Backup Slide 3) for cross-flows
  - Discharge calorimetry for global energy deposition measure
  - Time-resolved measure of spark channel temperature measurements (e.g., Rayleigh scatter)
- **GBDI discharge measurements**
  - Prototype new igniter variants & measure quantities of interest (e.g., O_3) at a broad range of pressures

- **Measurements of plasma-to-flame transition (e.g., number & size of kernels)**
  - Spark/LTP channel microscopy of flame kernel number, shape, and size distribution
- **Flame kernel wrinkling measurements to capture laminar-to-turbulent transition**
- **Prototype/test passive GBDI pre-chamber to leverage dilution tolerance benefits**

- **Spark retard limit testing at cold-start & high-load knock limited conditions using conventional SI and GBDI**
- **SACI with GBDI using pre-strikes to form O_3 (see Technical Backup Slide 1)**
- **Igniter prototype engine testing (performance/emissions/new combustion modes)**

Outcome: Proposed measurements are expected to lead to better *conventional spark* and *low-temperature plasma* ignition modeling for dilute/lean conditions

Any proposed future work is subject to change based on funding levels

Summary Slide

Relevance

- Improved ignition can enable a 25% increase in engine efficiency, lower pollutant emissions, and more reliable cold-start, but requires improved understanding and robust modeling approaches to optimize

Approach

- Couple unique capabilities to design/fabricate custom igniters and measure ignition quantities of interest with complementary engine testing

Technical Accomplishments (1/2)

- *GBDI Flame Growth Rate Measurements*: Extended ignition limits for lean (ϕ: 0.56 → 0.45) and dilute (EGR: 32% → 41%) mixtures, with early flame propagation rates that more than doubled
- *GBDI Igniter Development*: GBDI redesigned with a covered anode, which: (1) eliminated breakdown, (2) expanded lean ignition limits (ϕ: 0.45 → 0.41) , and (3) led to faster flame growth
- *GBDI O_3 formation*: GBDI discharge O_3 measured as a function of pulse energy/pressure

Technical Accomplishments (2/2)

- *GBDI Engine Testing*: GBDI increases dilution tolerance by enabling greater spark retard
- *O_3-enhanced SACI*:
  - *Stratified*: Broad range of possible loads/speeds; PM/NOx can be problematic.
  - *Homogeneous*: Limited to higher loads (> 4 bar IMEP) & lower speeds (< 1400 rpm); ultra-low PM/NOx
- *Kinetics of O_3 addition*: Impact of O made from O_3 pyrolysis on LTHR pathways explained

Proposed Future Research

- Conventional spark flame kernel microscopy
- Spark flame front wrinkling measurements
- Work w/ LLNL to model O_3 EGR interactions
- GBDI SACI to eliminate external O_3 formation (can we eliminate the need for the 2nd injection?)
- Plasma igniter prototype development/testing
- Ignition retard limits w/ spark & GBDI

The work was performed at the Combustion Research Facility, Sandia National Laboratories, Livermore, CA. Financial support was provided by the U.S. Department of Energy, Vehicle Technologies Office. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

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2019 DOE Vehicle Technologies Annual Merit Review
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June 11, 2019 – 9:30 a.m.

Program Managers: Michael R. Weismiller & Gurpreet Singh
U.S. DOE Office of Vehicle Technologies

Project ID: ACE006

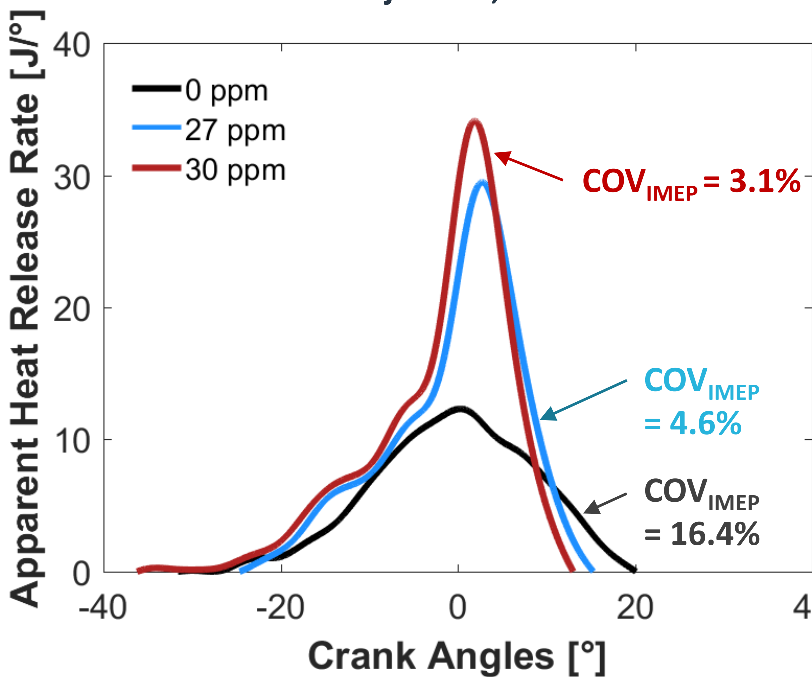
This presentation does not contain any proprietary, confidential, or otherwise restricted information

Technical Backup Slides

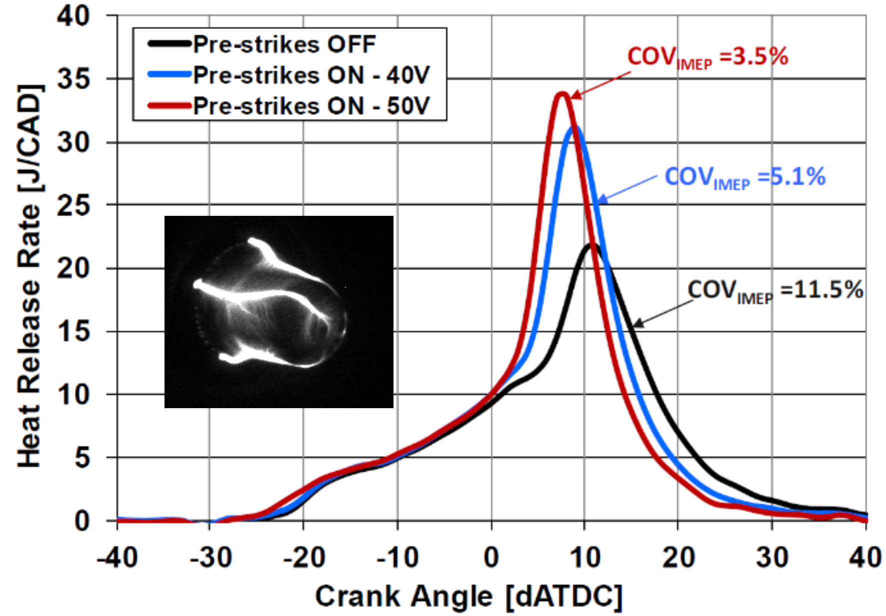
Technical Backup Slide

Heat release comparison: O_3-enhanced SACI Heat Release (SNL – ACE006)
GBDI ignition with pre-strikes (GM – ACE121)

1000 rpm, 11.8 mg/cycle, T_{intake} = 42 ^{0}C
18.2% fuel in 2nd injection, 93 mJ inductor coil spark



1000 rpm, 12 mg/cycle, T_{intake} = 40 ^{0}C
16.7% fuel in 2nd injection, GBDI igniter

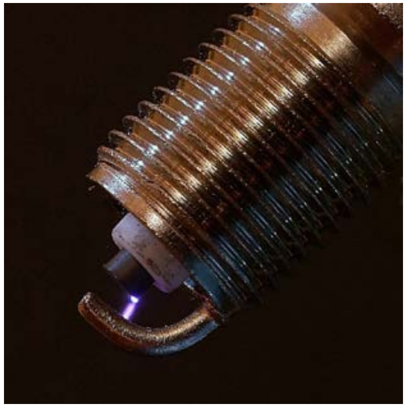


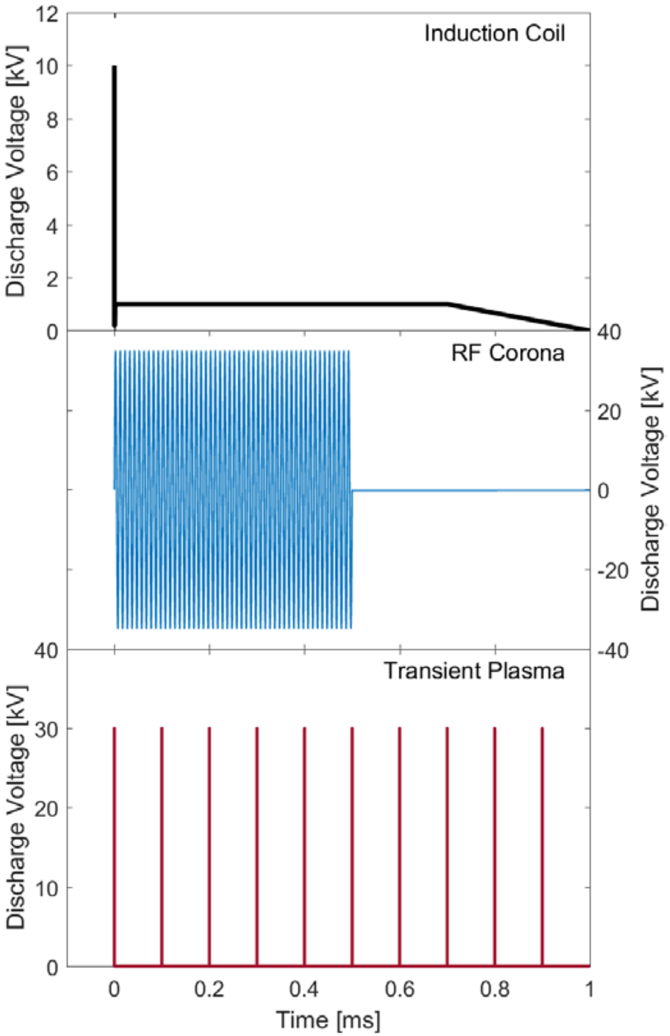
Cherian A. Idicheria, IAV Ignition Systems for Gasoline Engines conference, Berlin, 2018

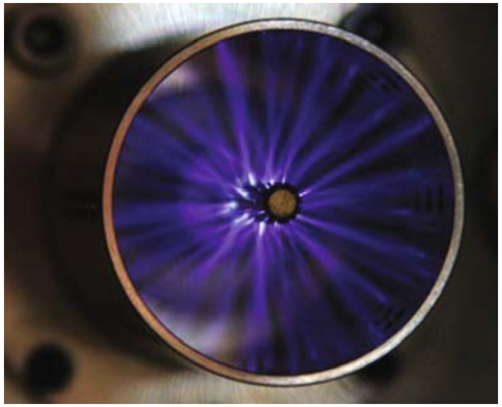
Impact: Good agreement between companion experiments show igniter O_3 formation is responsible for enhanced heat release & improved stability

Technical Backup Slide – Plasma Igniter Comparison

1. Inductive coil spark
   - Localized thermal plasma
2. Radio Frequency Corona
   - Distributed high-frequency breakdown
3. Transient Plasma Ignition
   - Short-pulse glow-phase ignition







Technical Backup Slide – Updates on other tasks

New Ignition Test Vessel

Done:
- Designed/fabricated vessel
- Installed custom windows
- Pressure tested completed assembly
- Initial testing of plasma igniters

To Do:
- Design modifications to enable cross (and swirl?) flows

Dynamic Skip Fire SG2 Head Modifications

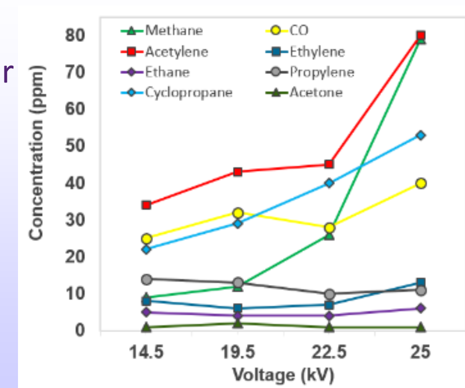
Done:
- Identified hardware (roller finger followers, oil control valves)
- Engineering analysis on head mods
- Updated head drawings

To Do:
- Head mods at external shop
- Design/build emissions sampling system for cycle resolved PM/PN measurements

Measure TPI Discharge Products

Done:
- Bulk sampling of fuel/air discharge products
- Discharge O_3 formation
- O-atom concentrations

To Do:
- Electron and bulk-gas temperatures



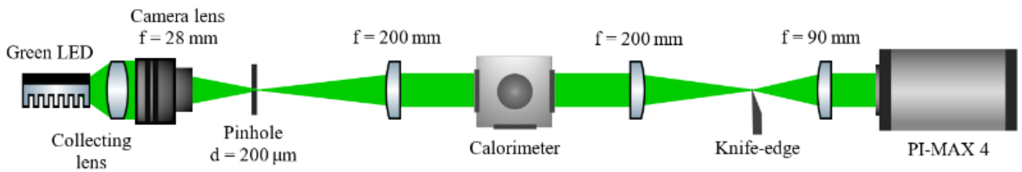
Pre-Chamber Igniter Prototypes

Done:
- Designed/built passive mode outer-body
- Designed active mode fueling ring

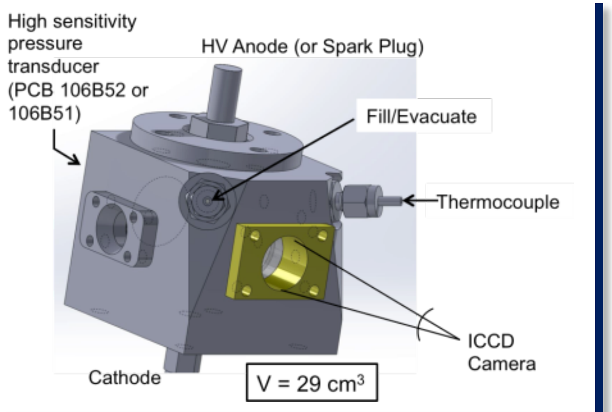
To Do:
- Complete/test active mode fueling ring
- Vessel/engine prototype testing for stoich, dilute, and lean combustion
- Develop plasma PC

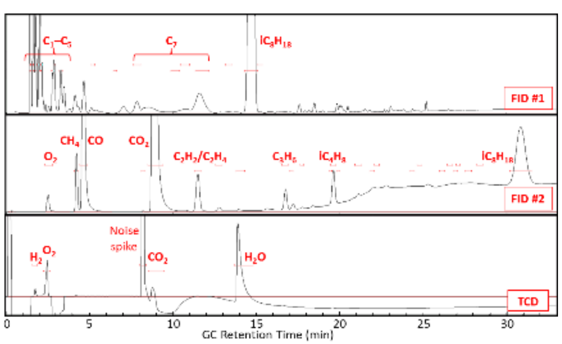
Goal: Eliminate active fueling while preserving lean/dilution tolerance

Technical Backup Slide – Diagnostics



Optical Ignition Calorimeter



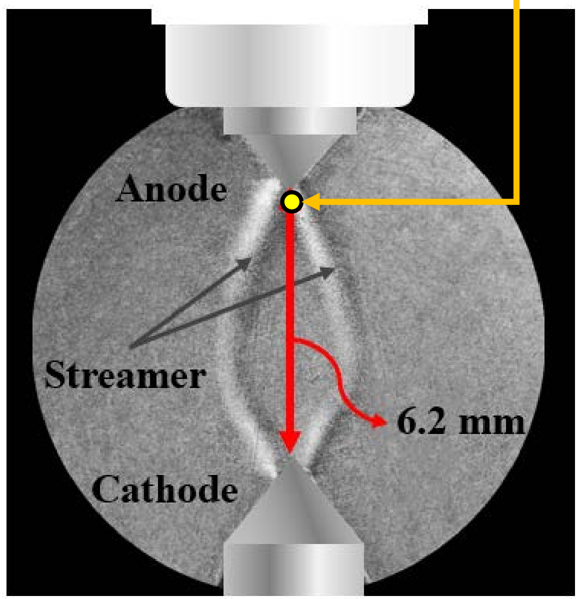


Gas chromatography

- Discharge generated radicals

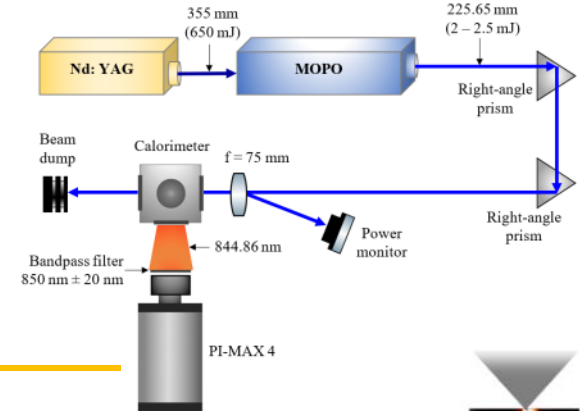
Schlieren imaging

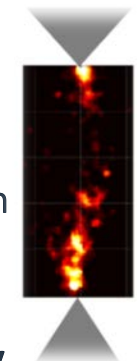
- Discharge volume
- Channel temperature (with calorimetry)
- Flame kernel growth



2-photon absorption laser induced fluorescence (TALIF) of O radical

- Quantitative O-atom conc.



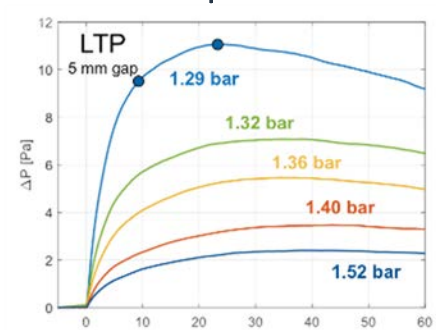


Filtered O* imaging

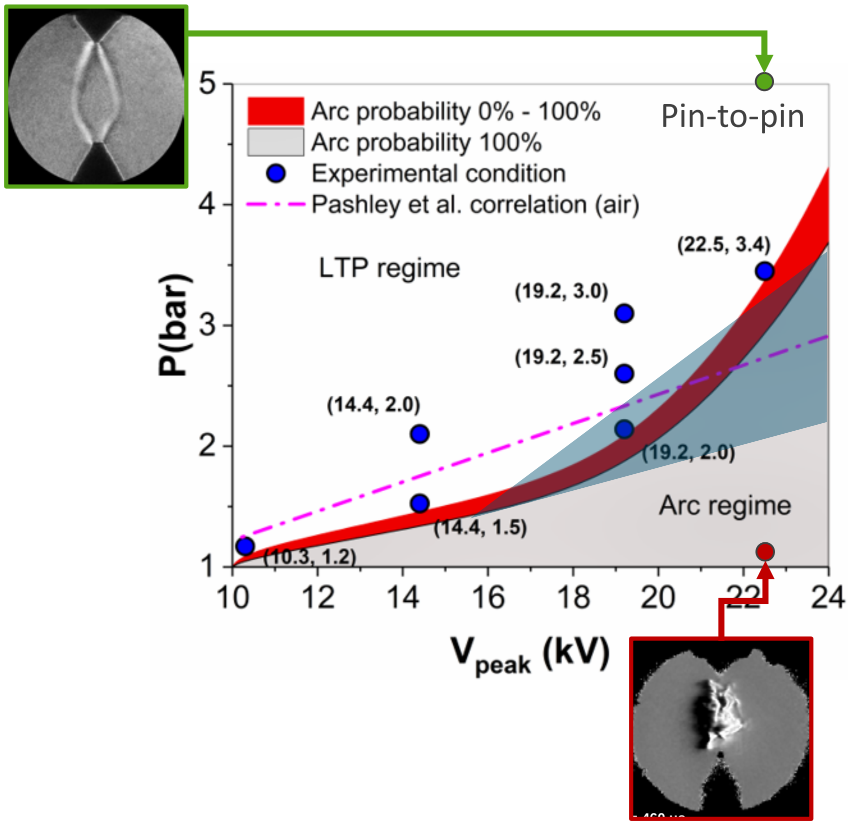
- Qualitative visualization of streamer structure

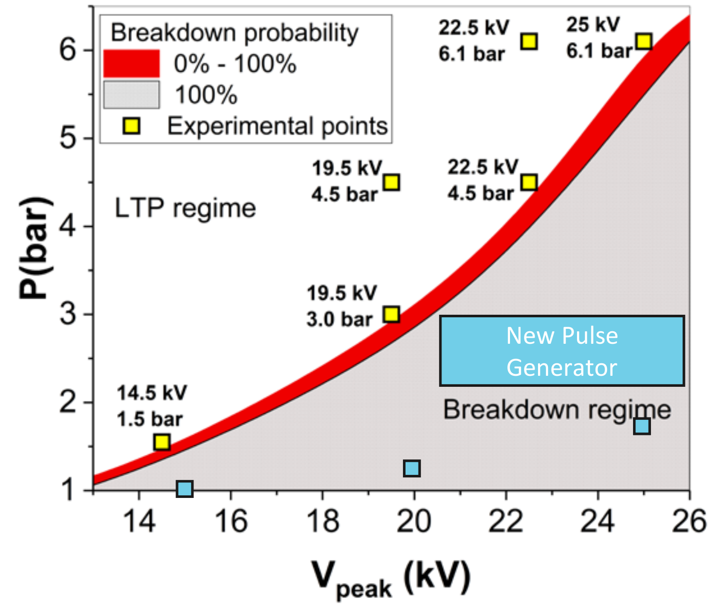
Pressure-rise calorimetry

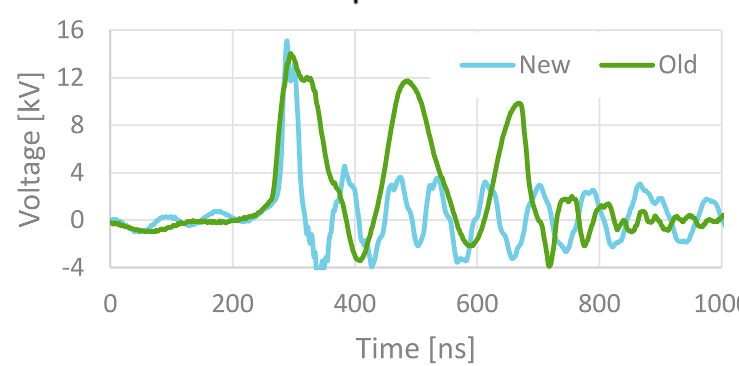
- LTP temperature



Technical Backup Slide – Improved pulse generator







Shorter pulses and better gas impedance matching helped to eliminate secondary breakdown issues